## => FILE REG

FILE 'REGISTRY' ENTERED AT 11:54:53 ON 26 AUG 2008
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## => D HIS

L1 L2 L3 L4		'HCA' ENTERED AT 11:42:26 ON 26 AUG 2008 77 S SURBURG ?/AU 2558 S ROHDE ?/AU 23012 S KOCH ?/AU 1 S L1 AND L2 AND L3 SEL RN
	FILE	'REGISTRY' ENTERED AT 11:42:55 ON 26 AUG 2008
L5		1 S 3664-64-0
L6		1 S 41096-60-0
		E $7-NONEN-2-ONE$ , $4,8-DIMETHYL-/CN$
L7		2 S E5 OR E6 OR E7 OR E8
L8		3 S L5 OR L7
		E 2-NONANONE, 4,8-DIMETHYL-/CN
L9		1 S E4 OR E5 OR E6
L10		2 S L6 OR L9
	FTLE	'ZCA' ENTERED AT 11:49:45 ON 26 AUG 2008
L11		46 S L8
L12		10 S L10
L13		2 S L11 AND L12
L14		8 S L12 NOT L13
L15		44 S L11 NOT (L13 OR L14)
L16		2 S 1840-2003/PY, PRY, AY AND L13
L17		8 S 1840-2003/PY, PRY, AY AND L14
L18		41 S 1840-2003/PY, PRY, AY AND L15

## => FILE ZCA

FILE 'ZCA' ENTERED AT 11:55:05 ON 26 AUG 2008
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# => D L13 1-2 BIB ABS HITSTR HITRN

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ANSWER 1 OF 2 ZCA COPYRIGHT 2008 ACS on STN
L13
ΑN
     142:140848
                ZCA
                     Full-text
     Use of 4.8-dimethyl-7-nonen-2-one and 4.8-dimethylnonan-2-one as
ΤI
     perfumes
     Surburg, Horst; Rohde, Ute; Koch, Oskar
ΙN
PA
     Symrise GmbH & Co. KG, Germany
SO
    PCT Int. Appl., 31 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     German
FAN.CNT 1
     PATENT NO.
                        KIND DATE APPLICATION NO.
                                                                  DATE
PΙ
    WO 2005004825
                        A1
                               20050120
                                          WO 2004-EP51112
                                                                  200406
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA,
         W:
             CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,
             GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP,
            KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW,
            MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD,
             SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ,
             VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
            AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,
             DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL,
            PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
             GW, ML, MR, NE, SN, TD, TG
                              20050127
     DE 10330865
                         Α1
                                          DE 2003-10330865
                                                                  200307
                                                                  09
    EP 1682230
                            20060726
                                        EP 2004-741800
                         Α1
                                                                  200406
                                                                  15
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC,
            PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
     US 20060166857
                         Α1
                            20060727 US 2006-563875
                                                                  200601
                                                                  09
PRAI DE 2003-10330865
                               20030709
                        A
    WO 2004-EP51112 W
                               20040615
```

The invention relates to the use of 4,8-dimethyl-7-nonen-2-one and 4,8-dimethylnonan-2-one as perfumes with a rose scent. The invention also relates to corresponding perfume compns., perfumed products and methods for creating or intensifying a rose scent. The perfumes can be added to cosmetic prepns. and to detergents. Thus 4,8-dimethyl-7-nonen-2-one and 4,8-dimethylnonan-2-one were prepd. by Raney-nickel hydrogenation of 4,8-dimethyl-3,7-nonadien-2-one. A perfume was prepd. from (w/%): 10-undecenal 2; Datilat 15; 9-decenol 1; eugenol 5; Guaiac wood oil 7; Indoflor 2;  $\alpha$ -ionone 20;  $\beta$ -ionone 7; cyclohexadecanone 17; 10% phenylacetaldehyde in dipropylene glycol 7; Pyroprunat 10; 10% rose oxide in dipropylene glycol; total 100 wt. parts; to this mixt. 125 wt. parts 4,8-dimethyl-7-nonen-2-one and 125 wt. parts 4,8-dimethylnonan-2-one were added.

IT 3664-64-0P, 4,8-Dimethyl-7-nonen-2-one 41096-60-0P, 4,8-Dimethylnonan-2-one (use of 4,8-di-Me-7-nonen-2-one and 4,8-dimethylnonan-2-one as perfumes)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

RN 41096-60-0 ZCA CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P, 4,8-Dimethyl-7-nonen-2-one 41096-60-0P, 4,8-Dimethylnonan-2-one (use of 4,8-di-Me-7-nonen-2-one and 4,8-dimethylnonan-2-one as perfumes)

L13 ANSWER 2 OF 2 ZCA COPYRIGHT 2008 ACS on STN

AN 129:27585 ZCA Full-text

OREF 129:5879a,5882a

TI Ruthenium-Catalyzed  $\beta$ -Allyl Elimination Leading to Selective Cleavage of a Carbon-Carbon Bond in Homoallyl Alcohols

- AU Kondo, Teruyuki; Kodoi, Kouichi; Nishinaga, Eiji; Okada, Takumi; Morisaki, Yasuhiro; Watanabe, Yoshihisa; Mitsudo, Take-aki
- CS Department of Energy and Hydrocarbon Chemistry Graduate School of Engineering, Kyoto University, Kyoto, 606-8501, Japan
- Journal of the American Chemical Society (1998), 120(22), 5587-5588 CODEN: JACSAT; ISSN: 0002-7863
- PB American Chemical Society
- DT Journal
- LA English
- AB RuCl2(PPh3)3 is a highly effective catalyst for the deallylation of tertiary homoallyl alcs. Under 10 atm of carbon monoxide at 180° in the presence of 5 mol % RuCl2(PPh3)3 catalyst and with an excess amt. of allyl acetate in THF, various tertiary homoallyl alcs. were converted to ketones and alkenes in high yields via selective cleavage of a C-C bond. For example, deallylation of 2-phenylpent-4-en-2-ol gave acetophenone in an isolated yield of 91% together with propene in 54% yield.
- IT 3664-64-0P

(ruthenium-catalyzed  $\beta$ -allyl elimination leading to selective cleavage of carbon-carbon bond in homoallyl alcs.)

- RN 3664-64-0 ZCA
- CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-

(ruthenium-catalyzed  $\beta$ -allyl elimination leading to selective cleavage of carbon-carbon bond in homoallyl alcs.)

- RN 41096-60-0 ZCA
- CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P

(ruthenium-catalyzed  $\beta\text{-allyl}$  elimination leading to selective cleavage of carbon-carbon bond in homoallyl alcs.)

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-

(ruthenium-catalyzed  $\beta$ -allyl elimination leading to selective cleavage of carbon-carbon bond in homoallyl alcs.) RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

## => D L14 1-8 BIB ABS HITSTR HITRN

L14 ANSWER 1 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 134:252075 ZCA Full-text

TI Synthesis of enantiopure homoallylic ethers by reagent controlled facial selective allylation of chiral ketones

AU Tietze, Lutz F.; Weigand, Berthold; Volkel, Ludwig; Wulff, Christian; Bittner, Christian

CS Institut fur Organische Chemie Georg-August-Universitat Gottingen, Gottingen, 37077, Germany

SO Chemistry--A European Journal (2001), 7(1), 161-168 CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 134:252075

GΙ

The stereoselective allylation of chiral Me ketones to give tertiary homoallylic ethers, which can easily be transformed into homoallylic alcs., is described. Reaction of the enantiopure ketones (I), (R)-Me2CH(CH2)3CH( $\beta$ Me)CH2COMe, (R)-MeCH( $\beta$ OSiPh2CMe3)CH2COMe, (S)-MeCH( $\alpha$ Ph)CH2COMe and the racemic ketones MeCH(OSiPh2CMe3)CH2COMe, MeCH(Ph)CH2COMe, MeCH2CH(Ph)COMe, MeCH2CH(Me)COMe with the norpseudoephedrine deriv. and allylsilane in the presence of a catalytic amt. of trifluoromethanesulfonic acid, led to a series of homoallylic ethers with good to excellent diastereoselectivity (85:15 to > 97:3). The allylation is reagent controlled and nearly independent from the stereogenic centers in the substrates. A

partial kinetic resoln. was obsd. using the racemic ketones. In the reaction of the chiral ketones with the achiral reagents ethoxytrimethylsilane and allylsilane only a low diastereoselectivity was obsd.

IT 76035-98-8P

(synthesis of enantiopure homoallylic ethers by reagent controlled facial selective allylation of chiral ketones)

RN 76035-98-8 ZCA

CN 2-Nonanone, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 76035-98-8P

(synthesis of enantiopure homoallylic ethers by reagent controlled facial selective allylation of chiral ketones)

RE.CNT 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 94:15877 ZCA Full-text

OREF 94:2667a,2670a

TI Catalytic extended double bond migration with retention of configuration: a "zip-reaction"

AU Weissberger, E.; Stockis, A.; Carr, D. D.; Giebfried, J.

CS Res. Lab., Eastman Kodak Co., Rochester, NY, 14650, USA

SO Bulletin des Societes Chimiques Belges (1980), 89(4), 281-7 CODEN: BSCBAG; ISSN: 0037-9646

DT Journal

LA English

AB Isomerizing (+)-citronellol in the presence of Fe(CO)5 gave (+)-dihydrocitronellol in 16±1% optical yield at 140°, presumably via a succession of 1,3-H shifts on the basis of isolated partially isomerized intermediates and isomerization products of deuterated citronellols. The obsd. partial retention of configuration suggests that metal-olefin dissocn. occurs after the completion of 1,7-isomerization.

IT 41096-60-0P 76035-98-8P

(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

RN 76035-98-8 ZCA

CN 2-Nonanone, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$Me_2CH$$
 (CH<sub>2</sub>)3 R Me  $Me$ 

IT 41096-60-0P 76035-98-8P (prepn. of)

L14 ANSWER 3 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 79:136237 ZCA Full-text

OREF 79:22081a,22084a

TI Stereochemistry of migrating carbon in Wagner-Meerwein rearrangement

AU Shono, T.; Fujita, K.; Kumai, S.

CS Dep. Synth. Chem., Kyoto Univ., Kyoto, Japan

SO Tetrahedron Letters (1973), (33), 3123-6 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

The optically active amine RCHMeCH2NH2 [R = Me2CH(CH2)3CHMe], prepd. in 5 steps from d-citronellal, was deaminated with HNO2 to give 11.8% RCH2CHMe2, 7.4% RCH(OH)Et, 73.4% RCHMeCH2OH, and 7.4% RCMe2OH. RCH2CHMe2 from migration of asym. C was oxidized to RCH2COMe whose optical activity was the same as the ketone prepd. from d-citronellal. Thus, the stereochem. of the migrating C was retained indicating a partial bonded transition state.

IT 41096-60-0P

(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P (prepn. of)

L14 ANSWER 4 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 78:136467 ZCA Full-text

OREF 78:21929a,21932a

TI Diolefinic aliphatic compounds

IN Henrick, Clive A.

PA Zoecon Corp.

SO Fr. Demande, 66 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.	CNT 4 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE –
ΡΙ	FR 2124279	A5	19720922	FR 1972-2777	197201 27
	FR 2124279 FR 2124279	A1 B1	19720922 19780203		2 /
	US 3752843	A	19730814	US 1971-187898	197110 08
	ZA 7107341	А	19730627	ZA 1971-7341	197111 02
	US 3816484	A	19740611	US 1971-201162	197111
	US 3824290	А	19740716	US 1971-206519	22 197112
	US 3855322	А	19741217	US 1971-206918	09 197112
	IL 38486	A	19750728	IL 1971-38486	10 197112 30

	ΑT	319910	В	19750110	ΑT	1972-317	
							197201
							14
	ΙT	972142	В	19740520	ΙT	1972-20052	100001
							197201 31
	шп	166175	В	19750128	штт	1972-Z0114	31
	110	100173	Ъ	19730120	110	19/2-20114	197201
							31
	RO	62770	A1	19780215	RO	1972-73287	
							197202
							15
	US	4021461	A	19770503	US	1972-265922	
							197206
		2022625	73	1074000		1070 20002	23
	US	3833635	A	19740903	US	1972-302983	197211
							01
	ΑТ	7400089	A	19751115	ΑТ	1974-89	O I
		7 10 0 0 0 0		13,01110		1371 03	197401
							07
	ΑT	331556	В	19760825			
	CA	1005823	A2	19770222	CA	1976-244761	
							197602
		4004 444600	_	40740004			02
PRAI		1971-111673	A	19710201			
		1971-111767 1971-187898		19710201 19711008			
		1971-111701	A2	1971000			
		1971-11673	A	19710201			
		1971-11701	A	19710201			
	US	1971-11767	А	19710201			
	CA	1971-127229	A3	19711109			
		1971-201102	A2	19711122			
		1972-317	A	19720114			
		1972-265922	A2	19720623			
AB	۱n	sacticidal alkadie	necarb	oxvlates wit	n i	uvenile hormone acti	771 T 77 -

Insacticidal alkadienecarboxylates with juvenile hormone activity, such as Me2CH(CH2)3CHMeCH2CH:CHCMe:CHCO2H (I) and its esters and amides were prepd. Thus Me2CH(CH2)3CHMeCH2-CHO was treated with MeCOCH2P(OEt)2 to give MeCOCH:-CHCH2CHMe(CH2)3CHMe2, which on treatment with EtO2C-CH2P(OEt)2 followed by hydrolysis of the ester gave I. The title compd. (I), useful as antiinflammatory drug and for the treatment of gastric ulcer, was prepd.in ~100% yield and increased purity by esterification of the alc. (II) under mild conditions with (PhCH2O2CCH2CH2CO)2O in pyridine or PhCH2O2-CCH2CH2COCl in pyridine-dioxane at 80-90° and room temp., resp., followed by hydrogenolytic PhCH2 group cleavage of III.

IT 41096-60-0P

(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P

(prepn. of)

L14 ANSWER 5 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 78:110633 ZCA Full-text

OREF 78:17759a,17762a

TI Aliphatic diolefins

IN Henrick, Clive A.

PA Zoecon Corp.

SO Ger. Offen., 94 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 4

r An .	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE -
PI	DE 2202016	А	19721123	DE 1972-2202016	197201 17
	DE 2202016 US 3752843	B2 A	19770811 19730814	US 1971-187898	197110 08
	ZA 7107341	А	19730627	ZA 1971-7341	197111 02
	CA 1005821	A1	19770222	CA 1971-127229	197111 09
	US 3816484	A	19740611	US 1971-201162	197111 22
	AU 7136208	А	19730531	AU 1971-36208	197111

GB	1368266	A	19740925	GB 1971-55200	26
GD	1300200	A	19740923	GB 1971-33200	197111 29
US	3824290	A	19740716	US 1971-206519	197112
US	3855322	A	19741217	US 1971-206918	09 197112
IL	38486	A	19750728	IL 1971-38486	10
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INL	7200032	A	19720003	NL 1972-032	197201 17
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	52005573	В	19770215		21
SE	385870	В	19760726	SE 1972-992	197201 28
СН	579526	A5	19760915	СН 1972-1265	197201
DD	100855	A5	19731012	DD 1972-160596	28
ΙT	972142	В	19740520	IT 1972-20052	197201 31
					197201 31
DD	107202	A5	19740720	DD 1972-165207	197201 31
DD	107850	A5	19740820	DD 1972-165190	197201
RO	62770	A1	19780215	RO 1972-73287	31 197202
US	4021461	A	19770503	US 1972-265922	15
					197206 23

	US	3833635	A	19740903	US 1972-302983	
						197211
				_		01
	ΑT	7400089	А	19751115	AT 1974-89	
						197401
	7	221556	D	10760005		07
		331556	В	19760825	TD 107E 22264	
	JP	51110512	А	19760930	JP 1975-22364	107500
						197502 21
	$C \Lambda$	1005823	A2	19770222	CA 1976-244761	21
	CA	1000020	AZ	19110222	CA 1970-244701	197602
						02
PRAT	US	1971-111673	А	19710201		0.2
		1971-111701	A	19710201		
		1971-111767	А	19710201		
	US	1971-187898	A	19711008		
	US	1971-11673	А	19710201		
	US	1971-11701	A	19710201		
	US	1971-11767	A	19710201		
	CA	1971-127229	A3	19711109		
	US	1971-201102	A2	19711122		
	ΑT	1972-317	A	19720114		
	US	1972-265922	A2	19720623		
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AB Alkadienyl acids, esters, nitriles, and amides were prepd. by treating an aldehyde or ketone with a phosphine or phosphono compd. contg. the corresponding acid deriv. Thus, MeCH2CHMe(CH2)3CHEtCH2CHO and (EtO)2P(O)CH2CMe:CHCO2Et in the presence of NaH gave E- and Z-EtO2CCH:CMeCH:CHCH2CHEt(CH2) 3CHMeCH2Me; (EtO)2P(O)CH2CN and MeCOCH:CHCH2CHMe(CH2)3CMe2Et in the presence of NaH gave E- and Z-Me2CEt(CH2)3CHMeCH2CH:CHCHMe:CHCN; and (EtO)2P(O)CH2CONEt2 and MeCOCH:CHCH2CHMe(CH2) 3CHMeEt gave E- and Z-EtCHMe(CH2) 3CHMeCH2CH:CHCONEt2. These products were converted by known methods to aldehydes, alcs., ethers, sulfides, and amines, and several were tested as insecticides.

IT 41096-60-0P

(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P (prepn. of)

L14 ANSWER 6 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 59:15934 ZCA Full-text

OREF 59:2925b-q

TI Amino sugar synthesis. XXV. Epimerization of N-substituted 2-amino-2-deoxyhexononitriles

AU Kuhn, Richard; Jochims, Johannes C.

CS Max Planck Inst. Med. Forsch., Heidelberg, Germany

SO Chemische Berichte (1963), 96, 983-9 CODEN: CHBEAM; ISSN: 0009-2940

DT Journal

LA Unavailable

GI For diagram(s), see printed CA Issue.

cf. CA 55, 27094b; 58, 12658f. Epimerization of N-substituted 2-AB amino-2-deoxyhexononitriles by heating in alcs. occurred by the reversible formation of HCN and pentosimines, and not via an intermediate imino lactone. 2-Deoxy-2-(diphenylmethylamino)-1-imino-D-galactono-1,4-lactone (I), m. 136-7° (C5H5N-Et2O),  $[\alpha]$ 19D -66° (c 1, C5H5N), was prepd. in 0.75-g. yield by shaking 1 g. 2-deoxy-2-(diphenylmethylamino) - D-galactononitrile (II) (obtained from the epimerie mixt. of 2-deoxy-2- (diphenylmethylamino)-D-galacto(D-talo)hexononitriles )(CA 55, 27089d) by fractional crystn., with 1% KOH in MeOH at 25° until dissolved, keeping at -25° for 3 h., filtering, washing with Et20, and purifying by dissolving in dry C5H5N and pptg. with Et20. The rotation of I changed rapidly in hot iso-PrOH with the formation of a brown sirup with no nitrile band in the IR spectrum. Thus, I is not an intermediate in the epimerization of II. (+) -3,7-Dimethyloctanal (III), b13 79-82°,  $[\alpha]$  20D 9.0°, was prepd. in 81% yield by hydrogenating (+)-3, 7-dimethyl-6-octenal over Pd-BaSO4 in 95% EtOH. (-)-3,7-Dimethyl-1-(9-fluorenylimino)octane (IV), m. 67-8°,  $[\alpha]$ 22D -2° (c 2.3, C5H5N), was prepd. in 20-g. crude yield by heating 20 g. III with an equimolar amt. of 9-aminofluorene in 40 cc. Et20 until a clear soln. was obtained, and crystq. the crude Schiff base from pentane. (-)-4,8-Dimethyl-2-(9fluorenylamino)nonanenitrile (V) (12.3 g.), m.  $64-6^{\circ}$  (sinters at 58°),  $[\alpha]$ 20D -55° (c 1.1, C5H5N), was obtained in 0.26-q. yield from 15 q. of purified IV dissolved in 100 cc. abs. EtOH, by introducing 15 cc. of anhyd. HCN at  $0^{\circ}$ , and keeping 24 h. at  $-78^{\circ}$ . (+)-4,8-Dimethyl-2- phenylaminononanenitrile (VI) (1.07 g.), m.  $62-4^{\circ}$ (pentane),  $[\alpha]$  22D 157° (c 1.0, MeOH),  $[\alpha]$  20D 164° (c 1.5, C5H5N), was obtained from 10 g. III and an equimolar amt. of PhNH2 in 20 cc. abs. EtOH, and the Schiff base, not isolated, treated with anhyd. HCN. Similarly, (-)-2-benzylamino-4,8- dimethylnonanenitrile hydrochloride (VII) (1.2 g.), m. 123-8° (PrOH),  $[\alpha]$ 20D -16° (c 1.1, MeOH),  $[\alpha]$ 25D

62° (c 2.0, C5H5N), was prepd. from 5 g. III by introducing HCl gas into an Et20 soln. of the sirupy amino nitrile. III (50 g.) in 50 cc. Et20 treated with MeMgI and the crude carbinol fractionally distd. gave 86% alc. (VIII), b13 102-6°, which (20 g.) was oxidized with 25 g. K2Cr2O7 in 20.5 g. H2SO4 and 125 cc. H2O to provide 17.5 g. (+)-4,8-dimethyl-2-nonanone (IX), b12-14 89-93°,  $[\alpha]$ 20D 3.02. (2.5 g.) dissolved in 2.6 g. 4-biphenylamine in 5 cc. HOAc was treated with 1 g. KCN in 1.5 cc. H2O, the mixt. shaken vigorously for 2 min., kept 10 h. at 10°, and the crude product recrystd. from pentane-methylcyclohexane, heptane-methyleyclohexane, and CHCl3pentane to give 1.3 g. (-)-2-(4-biphenylamino)-2,4,8trimethylnonanenitrile (X), m. 98-100°,  $[\alpha]$ 20D -41° (c 1.7, C5H5N). Equil. mixts. formed by dissolving 1 g. VI, X, or 2-benzylamino-2deoxy-D-glucononitrile (XI) in 100 cc. iso-PrOH to give HCN and Schiff bases were detd. by analyzing for HCN by addn. of AgNO3, filtration of AgCN, and titrn. with KSCN. Extent of dissocn. was given: (aminonitrile, temp., % dissocn.) VI, 30°, <1%; VI, 60°, 3%; VI, 80°, 4%; X, 30°, 33%; X, 45°, 50%; X, 60°, 58%; XI, 40°, 6%; XI, 65°, 10%; XI, 80°, 15%. Epimerization of N- substituted  $\alpha$ aminonitriles is thus not limited to sugar derivs.

IT 41096-60-0

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

$$\begin{array}{c} \begin{array}{c} \begin{array}{c} \text{O} & \text{Me} \\ \text{II} & \text{I} \end{array} \\ \text{Me-C-CH}_2\text{-CH-(CH}_2)} & 3\text{--CHMe} \end{array}$$

IT 76035-98-8P, 2-Nonanone, 4,8-dimethyl-, (+)-(prepn. of)

RN 76035-98-8 ZCA

CN 2-Nonanone, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 41096-60-0

(Derived from data in the 7th Collective Formula Index (1962-1966))

IT 76035-98-8P, 2-Nonanone, 4,8-dimethyl-, (+)- (prepn. of)

L14 ANSWER 7 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 52:65610 ZCA Full-text

OREF 52:11738a-b

TI Ketonization of dihydrocitronellic acid

AU Yeh, Ping-Yuan; Chow, Yuan-Lang

CS Natl. Taiwan Univ., Taipei, Taiwan

SO Perfumery and Essential Oil Record (1958), 49, 70-2 CODEN: PEORAA; ISSN: 0369-8998

DT Journal

LA Unavailable

AB Catalytic ketonization of dihydrocitronellic acid (I) by means of ferrous oxide catalyst gave 20% yield of 2,6,10,14-tetramethyl-8-pentadecanone. Pyrolysis of Ca, Ba, Fe++, and Pb dihydrocitronellates was also attempted. Pyrolysis of the Pb salt gave a satisfactory yield of I. 4,8-Dimethyl-2-nonanone was also prepd. by the Pb salt method.

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-

(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-(prepn. of)

L14 ANSWER 8 OF 8 ZCA COPYRIGHT 2008 ACS on STN

AN 47:41118 ZCA Full-text

OREF 47:6867d-i

TI Hydroxy fatty acids

AU Breusch, F. L.; Baykut, Fikret

CS Univ. Istanbul, Turk.

SO Rev. faculte sci. univ. Istanbul (1951), 16a, 137-43

DT Journal

LA German

cf. C.A. 46, 3946a. Some 2,3- and 3,5-HO fatty acids are prepd. by AB oxidn. of the unsatd. acid and the Reformatskii reaction with HO ketones, resp. BuCH: CHCO2H (2.6 g.), 4 g. Na2CO3, and 1.2 l. H2O below 10° were treated with 3.2 g. KMnO4 in 150 mL. H2O in 1 portion, and an excess of Na2SO3 and 10% H2SO4 was stirred in after 5 min., the soln. continuously extd. with ether for 2 days, the ether evapd., and the colorless crystals washed with petr. ether to yield 25% (crude) 2,3-dihydroxyheptanoic acid, m. 114-15° (from Me2CO-C6H6), sol. in alc. and Me2CO, insol. in petr. ether. 2,3-Dihydroxyoctanoic acid (15%), m. 118-19°, moderately sol. in H2O, 2,3-dihydroxytridecanoic acid, m. 126°, slightly sol. in C6H6, and 2,3-dihydroxy-5,9-dimethyldecanoic acid, (20%), m. 74.5-5.5°), were prepd. in the same manner. 5,9-Dimethyl-2-decenoic acid, b5 150-3°, [bis(p-dimethylaminophenyl)ureide, yellow crystals from alc., m. 112°], for the prepn of the corresponding dihydroxy acid was formed from CH2(CO2H)2 and 3,7-dimethyloctanol. C6H6 (10 mL.), 8.5 q. BrCH2CO2-Et, and 8.5 g. 4-hydroxy-2-decanone were added slowly with rapid stirring and initial heating to 3.5 g. Zn, the resulting ester treated with 3 g. KOH in 30 mL. EtOH 12 h. at room temp., 200 mL. H2O added, the soln. extd. 6 times with ether, the H2O layer was acidified with 10 % H2SO4, extd. with ether, and the ether washed with H2O, dried with Na2SO4, filtered, and evapd. to a colorless oil, 3,5-dihydroxy-3-methylundecanoic acid 5-lactone (pbromobenzylpseudothiuronium salt, colorless crystals, m. 132-3°). 3,5-Dihydroxy-3-methyldodecanoic acid 5-lactone, colorless oil (pbromobenzylpseudothiuronium salt, colorless crystals, m. 138°), 3hydroxy-3,5,9-trimethyldecanoic acid, colorless oil (70%) [bis(pdimethylaminophenyl)ureide, C30H46O3N4, colorless crystals from alc., m. 112°], and 3-hydroxy-2,3,5,9-tetramethyldecanoic acid, viscous colorless oil (50%), (p-bromobenzylpseudothiuronium salt, colorless crystals, m.  $113-14^{\circ}$ ), were prepd. in the same manner. Oxidn. of 80 g. tetrahydrogeraniol in 1 l. H2O at 10-20° with finely powd. KMnO4, bleaching with Na2SO3 in 10% H2SO4, and distn. gave 45 g. 3,7dimethyloctanoic acid; its Ba salt heated at 400° with 300 g. Ba(OAc)2 yielded 18 g. 4,8-dimethyl-2-nonanone, b45 130-3° (semicarbazone, colorless crystals from alc., m. 87°), which was used in the prepn. of the two 3-HO acids.

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-(prepn. of)

RN 41096-60-0 ZCA

CN 2-Nonanone, 4,8-dimethyl- (CA INDEX NAME)

IT 41096-60-0P, 2-Nonanone, 4,8-dimethyl-(prepn. of)

### => D L18 1-41 BIB ABS HITSTR HITRN

AB

ANSWER 1 OF 41 ZCA COPYRIGHT 2008 ACS on STN L18 141:350297 ZCA Full-text AN Process for producing (1R, 6R) - 2, 2, 6-trimethylcyclohexyl methyl TΙ ketone and/or (1R,6S)-2,2,6-trimethylcyclohexyl methyl ketone Ujihara, Hideo; Watanabe, Shinya; Yamamoto, Takeshi; Haqiwara, INPA Takasago International Corporation, Japan SO Eur. Pat. Appl., 18 pp. CODEN: EPXXDW Patent DTLA English FAN.CNT 2 KIND DATE APPLICATION NO. PATENT NO. DATE PIEP 1468978 A1 20041020 EP 2004-13984 200106 07 <--R: CH, DE, ES, FR, GB, LI, NL JP 2001348353 A 20011218 JP 2000-170822 200006 07 <--A2 20011212 EP 2001-401473 EP 1162191 200106 07 <--EP 1162191 A3 20020904 B1 20050629 EP 1162191 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO PRAI JP 2000-170822 A 20000607 <--A3 20010607 <--EP 2001-401473 OS MARPAT 141:350297

The invention relates to a process for producing (1S, 6R) - 2, 2, 6

trimethylcyclohexyl Me ketone from (3R) - or (3S) -citronellal. Thus,

trimethylcyclohexyl Me ketone and/or (1R,6S)-2,2,6-

(3S)-citronellal was converted to (4S)-4,8-dimethyl-2,7-(and 1,7)-nonadienyl-2-yl acetate which was cyclized to (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone (I). I was treated with EtMgCl and MeCHO to give (1R,6S)-(2,2,6-trimethylcyclohexyl)-2-buten-1-one. A unique, novel eucalyptus, mint-like and white floral perfume material can be provided using the prepd. ketone compds.

IT 82507-53-7P

(process for producing (1R,6R)-2, 2, 6-trimethylcyclohexyl Me ketone and/or (1R,6S)-2, 2, 6-trimethylcyclohexyl Me ketone)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7P

(process for producing (1R,6R)-2,2,6-trimethylcyclohexyl Me ketone and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 140:235334 ZCA Full-text

- TI Catalytic conversions in water. Part 23: Steric effects and increased substrate scope in the palladium-neocuproine catalyzed aerobic oxidation of alcohols in aqueous solvents
- AU ten Brink, Gerd-jan; Arends, Isabel W. C. E.; Hoogenraad, Marcel; Verspui, Goeran; Sheldon, Roger A.
- CS Laboratory for Biocatalysis and Organic Chemistry, Delft University of Technology, Delft, 2628 BL, Neth.
- SO Advanced Synthesis & Catalysis (2003), 345(12), 1341-1352 CODEN: ASCAF7; ISSN: 1615-4150
- PB Wiley-VCH Verlag GmbH & Co. KGaA
- DT Journal
- LA English
- OS CASREACT 140:235334
- AB The steric influence of substituents on the 2- and 9-positions of phenanthroline in the (2,9-R2-1,10-phenanthroline)palladium(II)-catalyzed aerobic oxidn. of 2-hexanol was investigated by means of high throughput experimentation. (Neocuproine)Pd-(OAc)2 (R=CH3) was found to be a highly active catalyst for alc. oxidn. in 1:1

water/DMSO mixts. The catalyst is unique in that it tolerates water, polar co-solvents and a wide variety of functional groups in the alc. Turn-over frequencies of  $> 1500\ h-1$  were achieved and a series of alcs. was oxidized with 0.1 to 0.5 mol % of catalyst.

IT 82507-53-7P

(steric effects and increased substrate scope in the palladium-neocuproine catalyzed aerobic oxidn. of alcs. in aq. solvents)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7P

(steric effects and increased substrate scope in the palladium-neocuproine catalyzed aerobic oxidn. of alcs. in aq. solvents)

RE.CNT 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 139:378160 ZCA Full-text

TI Insect chemistry and chirality

AU Hayes, Patricia Y.; Fletcher, Mary T.; Chow, Sharon; McGrath, Matthew J.; Tu, Yong Q.; Zhang, Hesheng; Hungerford, Natasha L.; McErlean, Christopher S. P.; Stok, Jeannette E.; Moore, Christopher J.; DeVoss, James J.; Kitching, William

CS Department of Chemistry, The University of Queensland, Brisbane, Australia

SO Chirality (2003), 15(Suppl.), S116-S127 CODEN: CHRLEP; ISSN: 0899-0042

PB Wiley-Liss, Inc.

DT Journal

LA English

AB Examn. of the chem. of a no. of Australian insect species provided examples of unusual structures and encouraged detns. of their abs. stereochem. by stereocontrolled syntheses and chromatog. comparisons. Inter alia, studies with the fruit-spotting bug (Amblypelta nitida), certain parasitic wasps (Biosteres sp.), the aposematic shield bug (Cantao parentum), and various species of scarab grubs are

summarized. The detn. of enantiomeric excesses (ee's) for component epoxides, lactones, spiroacetals, and allenes are described. Stereochem. and related aspects of the biosynthesis of spiroacetals in certain fruit-fly species (Bactrocerae sp.) are also presented.

IT 89272-56-0P

(in synthesis of insect hydrocarbons and assessment of chirality)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
 $R$ 
 $Me$ 
 $O$ 

IT 89272-56-0P

(in synthesis of insect hydrocarbons and assessment of chirality)
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 139:265438 ZCA Full-text

TI Preparation of a fragrance composition containing the isomers of optically active trans-1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one

IN Yamamoto, Takeshi; Wawtanabe, Shinya; Ujihara, Hideo; Hagiwara, Toshimitsu

PA Takasago International Corporation, Japan

SO Eur. Pat. Appl., 26 pp.

CODEN: EPXXDW

DT Patent

LA English

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US 20030207790	A1	20031106	US 2003-390733	200303 19

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US 6930083 B2 20050816

PRAI JP 2002-81953 A 20020322 <--

AB A geometrical isomer compn. excellent in odor and in chem. resistance, which is applicable to a base material contg. a strongly alk. chem. or a strongly acidic chem., which can suppress the deterioration with time and the color change of the base material in the case that the material is exposed to light, and which also have highly tasteful and unique fruity floral fragrance is disclosed. A geometrical isomer compn. contg. 93-99% of optically active trans-1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one (I) or a mixt. and 1-7% by wt. of optically active cis-1-(2,2,6-trimethylcyclohexyl)-2- buten-1-one or a mixt. is used. Thus, I was prepd. in a series of steps starting from optically active 4,8-dimethyl-7-nonen-2-ol. A formulation contained I 0.2, ammonium thioglycolate 10.0, aq. NH3 1.5, Nikkol BO-20 1.0, propylene glycol 5, sodium edetate 0.1, and water 88.2%.

IT 82507-53-7P

(prepn. of fragrance compn. contg. isomers of optically active trimethylcyclohexylbutenones)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7P

(prepn. of fragrance compn. contg. isomers of optically active trimethylcyclohexylbutenones)

L18 ANSWER 5 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 139:265437 ZCA Full-text

TI Preparation of a fragrance composition containing isomers of optically active ethyl trimethylcyclohexylcarboxylate

ΙN Yamamoto, Takeshi; Wawtanabe, Shinya; Ujihara, Hideo; Hagiwara, Toshimitsu

Takasago International Corporation, Japan PA

SO Eur. Pat. Appl., 24 pp.

CODEN: EPXXDW

Patent DT

English LA

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PRAI JP 2002-81954 Α

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A geometrical isomer compn. excellent in odor and in chem. resistance, which is applicable to a base material contq. a strongly alk. chem. or a strongly acidic chem., which can suppress the deterioration with time and the color change of the base material in the case that the material is exposed to light, and which also have highly palatable and unique fruity floral fragrance is disclosed. The compn. is produced by mixing 93-99% by wt. of optically active Et trans-2,2,6-trimethylcyclohexylcarboxylate (I) or a mixt. and 1-7% of optically active Et cis-2,2,6-trimethylcyclohexylcarboxylate or a mixt., resp. Thus, I was prepd. in a series of steps starting from (4S)-4,8-dimethyl-7-nonen-2-ol. A formulation contained I 3.0, NaOCl 4.0, PEG lauryl ether sulfate sodium salt 2.0, sodium 2-ethylhexyl sulfate 2.0, NaOH 1.0, I 0.1 and water qs to 100%.

82507-53-7P ΙT

> (prepn. of fragrance compns. contg. isomers of optically active Et trimethylcyclohexylcarboxylate)

82507-53-7 ZCA RN

7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME) CN

Absolute stereochemistry. Rotation (-).

$$Me_2C$$
  $Me$ 

IT 82507-53-7P

(prepn. of fragrance compns. contg. isomers of optically active Et trimethylcyclohexylcarboxylate)

L18 ANSWER 6 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 139:22084 ZCA Full-text

On the mechanism of carbohydroxypalladation of enynes. Additional insights on the cyclization of enynes with electrophilic metal complexes

AU Nevado, Cristina; Charruault, Lise; Michelet, Veronique; Nieto-Oberhuber, Cristina; Munoz, M. Paz; Mendez, Maria; Rager, Marie-Noelle; Genet, Jean-Pierre; Echavarren, Antonio M.

CS Departamento de Quimica Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain

SO European Journal of Organic Chemistry (2003), (4), 706-713 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

OS CASREACT 139:22084

GΙ

AB Different mechanisms have been proposed for the cyclization of enynes, e.g., I, catalyzed by electrophilic metal halides or complexes. We present evidence to indicate that the previously reported "carbohydroxypalladation" and the "hydroxycyclization catalyzed by PtII" are closely related reactions. Thus, palladium

complexes formed in situ from PdCl2 and trisulfonated phosphane TPPTS or cyclic phosphite P(OCH2)3CEt, as the ligands, catalyze the methoxy- or hydroxycyclization of enynes with selectivities similar to those obsd. with PtII complexes. Deuteration studies indicate that activation of the alkyne by PdII promotes an anti-addn. of the alkene.

IT 3664-64-0P, 4,8-Dimethyl-7-nonen-2-one (byproduct from the attempted methoxycyclization of dimethylnonenyne)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P, 4,8-Dimethyl-7-nonen-2-one (byproduct from the attempted methoxycyclization of dimethylnonenyne)

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 138:368540 ZCA Full-text

TI Synthesis and odor of optically active trans-2,2,6trimethylcyclohexyl methyl ketones and their related compounds

AU Yamamoto, Takeshi; Ujihara, Hideo; Watanabe, Shinya; Harada, Makoto; Matsuda, Hiroyuki; Hagiwara, Toshimitsu

CS Central Research Laboratory, Takasago International Corporation, Hiratsuka, Kanagawa, 254-0073, Japan

SO Tetrahedron (2003), 59(4), 517-524 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 138:368540

The syntheses of (1R,6S)-and (1S,6R)-2,2,6-trimethylcyclohexyl Me ketones (I) and (II) via cationic olefin cyclizations of ketone enol esters and their odor is described. (E)-(1R,6S)-and(E)-(1S,6R)-1-(2,2,6-trimethylcyclohexyl)-2-buten-1-one were prepd. via stereoselective aldol condensation of I and II, followed by dehydration. (1R,6S)-Et 2,2,6-trimethylcyclohexylcarboxylate was prepd. via stereoselective oxidn. of I.

IT 82507-53-7P

(synthesis and odor of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7P

(synthesis and odor of trimethylcyclohexyl ketones via cationic olefin cyclization, stereoselective aldol condensation, and stereoselective oxidn.)

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 8 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 137:47320 ZCA Full-text

TI Stereoselective Prins cyclizations of  $\delta$ , vepsiln.-unsaturated ketones to cis-3-chlorocyclohexanols with TiCl4

AU Davis, Chad E.; Coates, Robert M.

CS Department of Chemistry, University of Illinois, Urbana, IL, 61801, USA

SO Angewandte Chemie, International Edition (2002), 41(3), 491-493

CODEN: ACIEF5; ISSN: 1433-7851

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 137:47320

GΙ

TiCl4-mediated Prins cyclization of  $\delta$ , .vepsiln.- and .vepsiln.,  $\zeta$ -AB unsatd. ketones provides a simple stereoselective annulation method for construction of thermodynamically stable, tertiary cyclohexanols, e.g., I, with incorporation of a cis-chloro substituent. Alternatively, use of HCl in place of TiCl4 provided the transchlorohydrins with variable selectivity and higher proportions of undesired cyclic olefins.

3664-64-0P ΙT

> (stereoselective prepn. of chlorocyclohexanols via titanium catalyzed Prins cyclizations of  $\delta_{t}$  .vepsiln. - and .vepsiln., $\zeta$ - unsatd. ketones)

3664-64-0 ZCA RN

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

3664-64-0P ΙT

> (stereoselective prepn. of chlorocyclohexanols via titanium catalyzed Prins cyclizations of  $\delta_{t}$  vepsiln. - and .vepsiln., $\zeta$ - unsatd. ketones)

25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 41 ZCA COPYRIGHT 2008 ACS on STN L18

136:309698 ZCA Full-text ΑN

Preparation of 2,2,6-trimethylcyclohexyl trichloromethyl ketone and TΙ 2,2,6-trimethylcyclohexanecarboxylic acids

Harada, Mutsumi; Matsuda, Hiroyuki; Ujihara, Hideo; Watabe, Shinya; INYamamoto, Takeshi

Takasago Perfumery Co., Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 9 pp. SO

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	JP 2002114738	A	20020416	JP 2000-309192	

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PRAI JP 2000-309192 20001010 <-OS CASREACT 136:309698; MARPAT 136:309698
GI

The compds. I (R = H, C1-4 alkyl) are prepd. by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone with hypochlorites and decompn. of 2,2,6-trimethylcyclohexyl trichloromethyl ketone with MOR (M = alkali metal; R = H, C1-4 alkyl). (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone was oxidized with NaClO in the presence of NaOH and trioctylmethylammonium chloride in hexane at 60° for 24 h to give 60% (1R,6S)-2,2,6-trimethylcyclohexyl trichloromethyl ketone, which was treated with NaOH in the presence of NaClO and Bu4NCl and Na2SO4 at 60-100° for 8 h to give 96% (1R,6S)-2,2,6-trimethylcyclohexanecarboxylic acid.

IT 82507-53-7P

(prepn. of trimethylcyclohexyl trichloromethyl ketone and trimethylcyclohexanecarboxylic acids)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7P

(prepn. of trimethylcyclohexyl trichloromethyl ketone and trimethylcyclohexanecarboxylic acids)

L18 ANSWER 10 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 136:167525 ZCA Full-text

TI Preparation of 2,2,6-trimethylcyclohexanecarboxylic acid from 2,2,6-trimethylcyclohexyl methyl ketone

IN Harada, Mutsumi; Matsuda, Hiroyuki; Ujihara, Hideo; Watabe, Shinya; Yamamoto, Takeshi

PA Takasago Perfumery Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	 JP 2002053520	A	20020219	JP 2000-242570	
					200008 10

<--

PRAI JP 2000-242570

20000810 <--

OS CASREACT 136:167525

AB 2,2,6-Trimethylcyclohexanecarboxylic acid (I), useful as an intermediate for fragrant substances, is prepd. by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone (II). Thus, (1R,6S)-II was oxidized by HNO3 at 90° for 3 h in H2O to give 98% (1R,6S)-I.

IT 82507-53-7P

(prepn. of 2,2,6-trimethylcyclohexanecarboxylic acid by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone by HNO3)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$Me2C$$
  $Me$ 

IT 82507-53-7P

(prepn. of 2,2,6-trimethylcyclohexanecarboxylic acid by oxidn. of 2,2,6-trimethylcyclohexyl Me ketone by HNO3)

L18 ANSWER 11 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 136:37794 ZCA Full-text

TI Process for producing (1S, 6R) - and/or (1R, 6S) - 2, 2, 6-

containing them Ujihara, Hideo; Watanabe, Shinya; Yamamoto, Takeshi; Toshimitsu, ΙN Takasago International Corporation, Japan PAEur. Pat. Appl., 17 pp. SO CODEN: EPXXDW DT Patent LA English FAN.CNT 2 APPLICATION NO. PATENT NO. KIND DATE DATE \_\_\_\_\_ \_\_\_\_\_ \_\_\_\_ \_\_\_\_\_ EP 1162191 A2 20011212 EP 2001-401473 PI200106 0.7 <--EP 1162191 A3 20020904 В1 EP 1162191 20050629 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO 20011218 JP 2000-170822 JP 2001348353 Α 200006 07 <--US 20020042356 A1 20020411 US 2001-876883 200106 07 <--US 6770618 B2 20040803 EP 1468978 Α1 20041020 EP 2004-13984 200106 07 <--R: CH, DE, ES, FR, GB, LI, NL ES 2244567 Т3 20051216 ES 2001-401473 200106 07 <--PRAI JP 2000-170822 Α 20000607 <--EP 2001-401473 AЗ 20010607 <--CASREACT 136:37794 OS GΙ

trimethylcyclohexyl methyl ketone and perfume compositions

AB A process for producing trans-2,2,6-trimethylcyclohexyl Me ketone, which is the (1S,6R)-2,2,6-trimethylcyclohexyl Me ketone (I) and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone (II), is described. Thus, I was prepd. from (R)-citronellol via condensation with EtMgBr in THF, Jones oxidn. in MeCOMe, acetylation with isopropenyl acetate contg. p-MeC6H4SO3H and cyclization with 85% H3PO4 in PhMe. A unique, novel eucalyptus, mint-like and white floral perfume material can be provided using the ketone compds. disclosed in the present invention as well by the prodn. process disclosed therein.

IT 82507-53-7P, (4S)-4,8-Dimethyl-7-nonen-2-one (prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in perfumes and colognes)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$\operatorname{Me}_2\operatorname{C} = \operatorname{Me}_0$$

IT 82507-53-7P, (4S)-4,8-Dimethyl-7-nonen-2-one (prepn of (1S,6R)- and/or (1R,6S)-2,2,6-trimethylcyclohexyl Me ketone for use in perfumes and colognes)

L18 ANSWER 12 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 134:115792 ZCA Full-text

TI Synthesis and stereochemistry of insect derived spiroacetals with branched carbon skeletons

AU Tu, Yong Q.; Hubener, Achim; Zhang, Hesheng; Moore, Christopher J.; Fletcher, Mary T.; Hayes, Patricia; Dettner, Konrad; Francke, Wittko; McErlean, Christopher S. P.; Kitching, William

CS Department of Chemistry, The University of Queensland, Brisbane, 4072, Australia

SO Synthesis (2000), (13), 1956-1978 CODEN: SYNTBF; ISSN: 0039-7881

PB Georg Thieme Verlag

DT Journal

LA English

OS CASREACT 134:115792

AB About thirty constitutionally different spiroacetals have been characterized from insects but only three have branched carbon skeletons. Two are based on the 1,7-dioxaspiro[5.5]undecane system and are certain stereoisomers of the 2,4,8-tri-Me deriv., from the aposematic shield bug, Cantao parentum (White), and a 2,2,8-tri-Me deriv. from the rove beetle, Ontholestes murinus (L). The 1,6-dioxaspiro[4.5]decane system is represented by a stereoisomer of the 2,3,7-tri-Me deriv. in the Cantao species. The elucidation of their structures and stereochem. by spectroscopy, synthesis and enantioselective gas chromatog. is described.

IT 89272-56-0P

(prepn. and stereochem. of insect derived spiroacetals with branched carbon skeletons)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
 $R$ 
 $Me$ 
 $O$ 

IT 89272-56-0P

(prepn. and stereochem. of insect derived spiroacetals with branched carbon skeletons)

RE.CNT 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 13 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 131:101437 ZCA Full-text

TI Effect of extraction techniques on the chemical composition and antioxidant activity of Eucalyptus camaldulensis var. brevirostris leaf oils

AU Fadel, Hoda; Marx, Friedhelm; El-Sawy, Abdalla; El-Ghorab, Ahemd

CS Chemistry Flavor Aromatic Department, National Research Center, Cairo, Egypt

SO Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung A: Food Research and Technology (1999), 208(3), 212-216

CODEN: ZLFAFA; ISSN: 1431-4630

PB Springer-Verlag

DT Journal

LA English

The volatile oil compns. of Eucalyptus camaldulensis var. AB brevirostris leaves obtained by hydrodistn. (HD) and supercrit. fluid extn. methods (SFE) were analyzed qual. and quant. by GLC-MS. Ninety different components were sepd. and most of them identified. In both exts. the main constituents were found to be  $\beta$ -phellandrene (8.94 and 4.09%), p-cymene (24.01 and 10.61%), cryptone (12.71 and 9.82%) and spathulenol (14.43 and 13.14%). The yield of the monoterpene hydrocarbons in HD oil (0.288 g/100 g fresh leaves) was slightly higher compared with that in the SFE ext. (0.242 g/100 g fresh leaves). The SFE ext. possessed higher concns. of the sesquiterpenes, light oxygenated compds. and heavy oxygenated compds. than the HD oil. The relationship between the antioxidant activity and chem. compn. of the extd. oils was investigated. The significant amts. of p-cymen-7-ol and thymol are responsible for the antioxidative activity of both exts. The concn. of both compds., but esp. that of p-cymen-7-ol (2.25%), is higher in the SFE ext. This corresponds with the higher antioxidative activity of the SFE compared with the HD ext. P-cymen-7-ol, a compd. newly identified in leaves of Eucalyptus species, exhibited superior antioxidant activity in comparison with that of butylated hydroxyanisole.

IT 3664-64-0

(effect of extn. techniques on the chem. compn. and antioxidant activity of Eucalyptus camaldulensis var. brevirostris leaf oils)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(effect of extn. techniques on the chem. compn. and antioxidant activity of Eucalyptus camaldulensis var. brevirostris leaf oils)

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 14 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 123:8778 ZCA Full-text

OREF 123:1855a,1858a

TI Organoaluminum-promoted direct conversion of aldehydes to the

homologous ketones or oxiranes with diazoalkanes

AU Maruoka, Keiji; Concepcion, Arnel B.; Yamamoto, Hisashi

CS Sch. Eng., Nagoya Univ., Nagoya, 464-01, Japan

SO Synlett (1994), (7), 521-3 CODEN: SYNLES; ISSN: 0936-5214

DT Journal

LA English

OS CASREACT 123:8778

AB Organoaluminum-promoted single homologation of aliph. and arom. aldehydes with diazoalkanes has been described. Among various organoaluminum reagents, exceptionally bulky methylaluminum bis(2,6-di-tert-butyl-4-methylphenoxide) (MAD) is found to be highly effective for the selective transformation of aliph. aldehydes to homologous ketones, while aluminum tris(2,6-diphenylphenoxide) (ATPH) enables the conversion of various aldehydes to oxiranes with diazomethane.

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 15 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 122:290484 ZCA Full-text

OREF 122:52959a,52962a

TI From (R)-(+)-pulegone to (2S,4R,6R,8S)-2,4,8-trimethyl-1,7-dioxaspiro[5.5]undecane - a unique spiroacetal from the insect kingdom

AU Tu, Yong Q.; Moore, Christopher J.; Kitching, William

CS Dep. Chem., Univ. Queensland, Brisbane, 4072, Australia

SO Tetrahedron: Asymmetry (1995), 6(2), 397-400 CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier

DT Journal

LA English

OS CASREACT 122:290484

AB Enantioselective synthesis of the unique, insect-derived spiroacetal, (2S, 4R, 6R, 8S)-2, 4, 8-trimethyl-1, 7- dioxaspiro[5.5] undecane and some

diastereomers, utilizing (R)-(+)-pulegone as chiral source-material, and asym. dihydroxylation as a key step, are described.

IT 89272-56-0P

(stereoselective prepn. of trimethyldioxazsiroundecane from pulegone)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me2C$$
 $R$ 
 $Me$ 

IT 89272-56-0P

(stereoselective prepn. of trimethyldioxazsiroundecane from pulegone)

L18 ANSWER 16 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 122:265067 ZCA Full-text

OREF 122:48389a,48392a

TI Synthesis and bioassay of all four stereoisomers of (2E,4E)-4,6,10,12-tetramethyl-2,4-tridecadien-7-one, the assignment of the absolute configuration of the sex pheromone of Matsucoccus matsumurae Japanese pine bast scale

AU Lin, Guo-Qiang; Xu, Wei-Chu; Qi, Yun-Tai; Chen, Guo-Min

CS Shanghai Institute Organic Chemistry, Chinese Academy Sciences, Shanghai, 200032, Peop. Rep. China

SO Chinese Journal of Chemistry (1995), 13(1), 85-94 CODEN: CJOCEV; ISSN: 1001-604X

PB Science Press

DT Journal

LA English

AB A facile enantioselective synthesis of all four stereoisomers of (2E,4E)-4,6,10,12-tetramethyl-2,4-tridecadien-7-one (I) is described. The stereochem. at C-6 and C-10 of I was constructed by using optically active citronellal as starting material and by the asym. crotylic metal reaction. In the bioassay and field tests, only (6R,10R)-I was active. The other three isomers were inactive. Therefore, the naturally occurring pheromone was assigned as (6R,10R)-I.

IT 89272-56-0P

(synthesis and pheromone activity of all four stereoisomers of (2E, 4E)-4, 6, 10, 12-tetramethyl-2,4-tridecadien-7-one)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
 $R$ 
 $Me$ 
 $O$ 

IT 89272-56-0P

(synthesis and pheromone activity of all four stereoisomers of (2E, 4E)-4, 6, 10, 12-tetramethyl-2,4-tridecadien-7-one)

L18 ANSWER 17 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 122:55346 ZCA Full-text

OREF 122:10727a,10730a

TI Regio- and stereoselective hydrogenation of conjugated carbonyl compounds via palladium assisted hydrogen transfer by ammonium formate

AU Ranu, Brindaban C.; Sarkar, Arunkanti

CS Department of Organic Chemistry, Indian Association for the Cultivation of Science, Calcutta, 700 032, India

SO Tetrahedron Letters (1994), 35(46), 8649-50 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier

DT Journal

LA English

OS CASREACT 122:55346

AB Excellent regio- and stereoselectivity has been achieved by using ammonium formate/Pd-C in the hydrogenation of the C=C bond conjugated to carbonyl group in presence of olefin.

IT 3664-64-0P, 7-Nonen-2-one, 4,8-dimethyl-

(regio- and stereoselective hydrogenation of conjugated carbonyl compds. via palladium assisted hydrogen transfer by ammonium formate)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P, 7-Nonen-2-one, 4,8-dimethyl-(regio- and stereoselective hydrogenation of conjugated carbonyl compds. via palladium assisted hydrogen transfer by ammonium formate)

L18 ANSWER 18 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 120:134079 ZCA Full-text

OREF 120:23599a,23602a

TI Enantioselective synthesis of all four stereoisomers of (2E,4E)-4,6,10,12-tetramethyl-2,4-tridecadien-7-one, the sex pheromone of Matsucoccus pine bast scale

AU Lin, Guogiang; Xu, Weichu

CS Shanghai Inst. Org. Chem., Chin. Acad. Sci., Shanghai, 200032, Peop. Rep. China

SO Tetrahedron Letters (1993), 34(37), 5931-4 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 120:134079

GΙ

AB A facile enantioselective synthesis of all four stereoisomers of (2E,4E)-4,6,10,12-tetramethyl-2,4-tridecadien-7-one (I) (6R,10R;6S,10R;6S,10S;6S,10S), the primary sex pheromone of Matsucoccus pine bast scale is described. The stereochem. at C-6 and C-10 of I was constructed by using optically active citronellal as starting material and by the asym. aldol reaction of (R)-heptanal II or its S isomer with (E)- and (Z)-boronates III.

IT 89272-56-0P

(intermediate in enantioselective synthesis of tetramethyltridecadienone stereoisomers)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
 $R$ 
 $Me$ 
 $O$ 

IT 89272-56-0P

(intermediate in enantioselective synthesis of tetramethyltridecadienone stereoisomers)

L18 ANSWER 19 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 116:194598 ZCA Full-text

OREF 116:32989a,32992a

TI The acid-catalyzed cyclizations of unsaturated carbonyl compounds utilizing silica gel at high pressure

AU Dauben, William G.; Hendricks, Robert T.

CS Dep. Chem., Univ. California, Berkeley, CA, 94720, USA

SO Tetrahedron Letters (1992), 33(5), 603-6

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA English

OS CASREACT 116:194598

GΙ

The ene-like cyclizations of a series of unsatd. carbonyl compds. were studied using silica gel at high pressure (15 kbar) as a new catalytic system. This new method is general for forming 5- and 6-membered ring carbocycles. Thus, treating R1CH2CHMeCH2CH2CH:CR2Me (R1 = CHO, R2 = Me) with silica gel 48h at 25° and 15 kbar gave 58% menthadienes I (R3 = OH, R4 = H, R5 = Me) and 15% I (R3 = H, R4 =

OH, R5 = Me); similarly, R1CHMeCH2CH2CH:CMe2 (R = CHO) gave 14% cyclopentanes II (R2 = Me, R3 = R5 = H, R4 = OH), 26% II (R2 = R5 = H, R3 = Me, R4 = OH), and 38% II (R2 = Me, R3 = R4 = H, R5 = OH). The mildness of this method was demonstrated by the successful cyclization of a vinyl cyclopropyl aldehyde.

IT 3664-64-0

(cyclization of, by silica gel at high pressure, menthenols from)  ${\tt RN} - 3664 - 64 - 0 - {\tt ZCA}$ 

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(cyclization of, by silica gel at high pressure, menthenols from)

L18 ANSWER 20 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 115:231928 ZCA Full-text

OREF 115:39513a,39516a

TI Synthetic Microbial Chemistry XXIV.-Synthesis of antibiotic 1233A, an inhibitor of cholesterol biosynthesis

AU Mori, Kenji; Takahashi, Yoshio

CS Dep. Agric. Chem., Univ. Tokyo, Tokyo, 113, Japan

SO Liebigs Annalen der Chemie (1991), (10), 1057-65 CODEN: LACHDL; ISSN: 0170-2041

DT Journal

LA English

OS CASREACT 115:231928

AB A synthesis of antibiotic 1233A (I) was achieved by employing (R)-HOCH2CH(CH2OAc)CH:CH2 and (R)-citronellic acid as chiral building blocks. The former was prepd. by lipase-mediated asym. hydrolysis of its diacetate.

IT 89272-56-0P

(prepn. and ketalization of)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
  $R$   $Me$ 

IT 89272-56-0P

(prepn. and ketalization of)

L18 ANSWER 21 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 112:158654 ZCA Full-text

OREF 112:26827a,26830a

TI Halogen effect on the ring opening of pulegone hydrohalides

AU Shull, Brian K.; Koreeda, Masato

CS Dep. Chem., Univ. Michigan, Ann Arbor, MI, 48109, USA

SO Journal of Organic Chemistry (1990), 55(7), 2249-51

CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 112:158654

AB Treatment of pulegone hydrohalides I (R = Cl, Br, iodo) with LiAlH4 gave (R)-(+)-citronellol (II) in 16%, 45%, and 60% yield, resp., whereas treatment of I (R = Cl, Br, iodo) with DIBAL gave II in 79%, 59% and 0% yield, resp. With the exception of LiAlH4, the yields of the ring-opening products with non-carbon nucleophiles decreased as the at. wt. of the starting hydrohalide halogen increased. A variety of carbon nucleophiles also cause a similar ring-opening reaction of the pulegone hydrohalides. With carbon nucleophiles, I (R = Cl) gave the best yield for the formation of the ring-opened products III (R1 = Me, Bu, CMe3, Ph), whereas treatment of I (R = iodo) with MeLi, BuLi, and PhLi gave mixts. of pulegone and the bis-adducts IV (R1 = Me, Bu, Ph). The relative propensity of I (R = Br, iodo) for ring opening of the initial mono-adduct contributes to the greater formation of bis-adducts with the exception of the reaction with t-BuLi.

IT 89272-56-0P

(prepn. of, via ring cleavage of pulegone hydrohalides by methyllithium)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
  $R$   $Me$ 

IT 89272-56-0P

(prepn. of, via ring cleavage of pulegone hydrohalides by methyllithium)

L18 ANSWER 22 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 112:115758 ZCA Full-text

OREF 112:19535a,19538a

TI Chemical constituents of the volatile oil of fresh flowers of Elaeagnus angustifolia L

AU Li, Zhaolin; Chen, Ning; Xue, Dunyuan; Li, Haiquan; Chen, Yaozu

CS Anal. Test. Cent., Lanzhou Univ., Lanzhou, Peop. Rep. China

SO Gaodeng Xuexiao Huaxue Xuebao (1989), 10(8), 804-8 CODEN: KTHPDM; ISSN: 0251-0790

DT Journal

LA Chinese

AB The essential oil of fresh flowers of E. angustifolia was extd. by simultaneous steam distn.—solvent extn. The yield of the oil was 0.1% of fresh flowers. By using capillary gas chromatog.—mass spectrometry, 85 constituents were sepd., of which 47 compds. constituting 96.51% of the oil were identified. The major ingredient was trans—ethyl cinnamate, accounting for ≤78.88% of the oil.

IT 3664-64-0

(from Elaeagnus angustifolia flower oil)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(from Elaeagnus angustifolia flower oil)

L18 ANSWER 23 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 111:232410 ZCA Full-text

OREF 111:38597a,38600a

TI Total synthesis of L-659,699, a novel inhibitor of cholesterol biosynthesis

AU Chiang, Yuan Ching P.; Yang, Shu Shu; Heck, James V.; Chabala, John C.; Chang, Michael N.

CS Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA

SO Journal of Organic Chemistry (1989), 54(24), 5708-12 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 111:232410

AB The total synthesis of L-659,699 (I) has been accomplished from pulegone. A key step involves a highly diastereoselective aldol condensation of chiral crotonate imide to introduce the stereogenic centers at the ring carbons.

IT 89272-56-0P

(prepn. and ketalization of)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

$$Me_2C$$
 $R$ 
 $Me$ 

IT 89272-56-0P

(prepn. and ketalization of)

L18 ANSWER 24 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 105:97701 ZCA Full-text

OREF 105:15797a,15800a

TI Syntheses and growth retarding activity of trialkylammonium compounds from citronellal

AU Sharma, M. L.; Pandhi, S. B.; Talwar, K. K.; Kalsi, P. S.

CS Dep. Chem., Punjab Agric. Univ., Ludhiana, 141 004, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(5), 571-3 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 105:97701

N,N,N-Trimethyl-5,9-dimethyl-2,8-decadienylammonium iodide, N,N,N-trimethyl-2,5,9-trimethyl-2,8-decadienylammonium iodide, N,N-diethyl-N-methyl-, N,N,N-triethyl-, and N,N-diethyl-N-butyl-3,7-dimethyl-6-octenylammonium iodide, N,N-diethyl-N-methyl-3,7-dimethyl-6-octenylammonium cyanide, and N,N,N-trimethyl-1,3,7-trimethyl-6-octenylammonium iodide were prepd. and examd. as plant growth retardants. These compds. inhibit root formation in hypocotyl cuttings of Phaseolus aureus.

IT 3664-64-0P

(prepn. and conversion of, into dimethylamino deriv.)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P

(prepn. and conversion of, into dimethylamino deriv.)

L18 ANSWER 25 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 100:121365 ZCA Full-text

OREF 100:18477a,18480a

TI Transformations of (+)-citronellal into insecticidal esters related to cut-up chrysanthemates

AU Randad, R. S.; Kulkarni, G. H.

CS Natl. Chem. Lab., Pune, 411 008, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1983), 22B(8), 795-801 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

AB (R)-RO2CCH2CH2CHMeCH:CR1R2 (I, R-R2 = Me, Me, Cl; Me, Ph, Cl; Me, Ph, H; Me, Me, Me), bearing close resemblance to chrysanthemates, were prepd. from (+)-citronellal and then converted by transesterification to the corresponding 3-phenoxybenzyl esters I (R = CH2C6H4OPh-m).

IT 89272-56-0P

(prepn. of, as intermediate for chrysanthemate analogs)

RN 89272-56-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4R)- (CA INDEX NAME)

Absolute stereochemistry.

IT 89272-56-0P

(prepn. of, as intermediate for chrysanthemate analogs)

L18 ANSWER 26 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 97:181446 ZCA Full-text

OREF 97:30341a,30344a

TI Alkylaluminum halide induced cyclization of unsaturated carbonyl compounds

AU Snider, Barry B.; Karras, Michael; Price, Robert T.; Rodini, David J.

CS Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA

SO Journal of Organic Chemistry (1982), 47(23), 4538-45 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 97:181446

2,6-Dimethyl-5-heptenal (I) and 5-octenal undergo concerted ene reactions with 1 equiv of Me2AlCl and cation-olefin cyclizations with 2 equiv of MeAlCl, MeAlCl2, or EtAlCl2 to give a zwitterion, which reacts to give several products including an ene adduct. 3,7-Dimethyl-6-octenal (II) and (Z)- and (E)-6-nonenal undergo only ene reactions with all catalysts. Me2C:CHCH2CH2CHMe(CH2)nCH:CHCOMe (n = 0, 1), formed by reaction of I and II with acetonylidenetriphenylphosphorane, react analogously to I and II in the presence of a Lewis acid. The effect of ring size on the nature of these cyclizations is explained on the basis of thermodn. and kinetic data.

IT 3664-64-0

(cyclization of, with alkylaluminum compds.)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(cyclization of, with alkylaluminum compds.)

L18 ANSWER 27 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 97:55328 ZCA Full-text

OREF 97:9305a,9308a

TI Synthesis of chiral cyclopentenoids

AU Drtina, Gary J.; Wiemer, David F.

CS Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA

SO Tetrahedron Letters (1982), 23(8), 803-6

CODEN: TELEAY; ISSN: 0040-4039

DT Journal

AB The methylcyclopentene I, a potential synthon in the prepn. of several diterpenoids, was prepd. from (-)-citronellal, with retention of the chiral center, by sequential Grignard reaction with H2C:CBrEt, oxidn., ozonolysis, cyclization, and ozonolysis.

IT 82507-53-7

(ozonolysis and redn. of)

RN 82507-53-7 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl-, (4S)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 82507-53-7

(ozonolysis and redn. of)

L18 ANSWER 28 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 96:122870 ZCA Full-text

OREF 96:20181a,20184a

TI Trialkylsilyl triflate in organic synthesis. 12. Ring opening of oxiranes by trimethylsilyl trifluoromethanesulfonate

AU Murata, Sizuaki; Suzuki, Masaaki; Noyori, Ryoji

CS Dep. Chem., Nagoya Univ., Nagoya, 464, Japan

SO Bulletin of the Chemical Society of Japan (1982), 55(1), 247-54

CODEN: BCSJA8; ISSN: 0009-2673

DT Journal

LA English

CASREACT 96:122870

OS GI

Me3SiOSO2CF3 (I) promotes ring opening reactions of oxirane derivs. AB The reaction course is highly affected by the structures and substitution pattern of the substrates. Tetra-, tri-, and 2,2substituted oxiranes and simple cycloalkene oxides are converted to the corresponding allylic alc. trimethylsilyl ethers, e.g., II. The overall transformation is interpreted in terms of trans addn. of I to the oxirane ring followed by base-promoted anti elimination of a trifluoromethanesulfonic acid element. 2,3-Dialkyl- or monoalkyloxiranes isomerize to the corresponding ketones and aldehydes, resp. (Z)-Cyclooctene oxide undergoes the transannular reaction to give endo-cis-2-trimethylsiloxybicyclo[3.3.0]octane. The reaction of 6-methyl-5-hepten-2-one oxide produces 2,2,6-trimethyl-3trimethylsiloxy-3,4-dihydro-2H-pyran. 1,2-Me migration takes place in the reaction of (E)-3 $\alpha$ -tert-butyldimethylsiloxy-5 $\alpha$ -pregnene  $17\alpha$ , 20-oxide to afford  $3\alpha$ -tert-butyldimethylsiloxy- $17\beta$ -methyl- $17\alpha$ -[1-(trimethylsiloxy)ethyl]-18-nor-5 $\alpha$ -androst-13(14)-ene.  $\alpha$ -Pinene oxide gives trans-carveol trimethylsilyl ether.

IT 3664-64-0P

(prepn. and epoxidn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. and epoxidn. of)

L18 ANSWER 29 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 95:187431 ZCA Full-text

OREF 95:31285a,31288a

TI Radical cyclizations of unsaturated aldehydes

AU Chatzopoulos, M.; Montheard, J. P.

CS Lab. Chim. Org., Unites Enseign-Rech. Sci., Saint-Etienne, 42023, Rom.

SO Revue Roumaine de Chimie (1981), 26(2), 275-82 CODEN: RRCHAX; ISSN: 0035-3930

DT Journal

LA French

GΙ

AB Ethylenic aldehydes underwent free radical cyclization to give ketones; thus, I yielded II and Me2C:CHCH2CH2CMe(CH:CH2)CH2CHO gave III and IV when cyclized in the presence of Me3COOCMe3 or (BzO)2. In cases where there was a choice between the formation of a cyclohexanone or cyclopentanone, the carbonyl radical added to the double bond to form a cyclohexanone ring. Thus, Me2C:CHCH2CH2CHMeCHO cyclized to give V.

IT 3664-64-0

(cyclization of, in presence of di-tert-butylperoxide)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(cyclization of, in presence of di-tert-butylperoxide)

L18 ANSWER 30 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 94:46816 ZCA Full-text

OREF 94:7625a,7628a

TI Alkylaluminum chloride induced cyclization of unsaturated carbonyl compounds

AU Karras, Michael; Snider, Barry B.

CS Dep. Chem., Princeton Univ., Princeton, NJ, 08544, USA

SO Journal of the American Chemical Society (1980), 102(27), 7951-3

CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA English

GΙ

$$\begin{array}{c} \stackrel{\text{Me}}{\longleftarrow} \stackrel{\text{A}\overline{\text{I}}\text{Me}_2\text{Cl}}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{CH}_2}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \\ \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longrightarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longrightarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longleftarrow} \stackrel{\text{H}}{\longrightarrow} \stackrel{\text{H}$$

2,6-Dimethyl-5-heptenal undergoes a concerted ene reaction with 1 equiv. of Me2AlCl at -80° to give I and a cation-olefin cyclization with 2 equiv. of Me2AlCl, MeAlCl2, or EtAlCl2 to give a zwitterion II (R = Me, Et; n = 1,2) whose further reactions depend on the Lewis acid used and the temp. 6,7-Unsatd. ketones undergo ene reactions with Me2AlCl as catalyst whereas 4,5- and 5,6-unsatd. ketones undergo cation-olefin cyclization with 2 equiv. of MeAlCl2 to give a zwitterion which undergoes a 1,2-hydride shift, followed by a 1,2-Me shift, to give a cyclopentanone.

IT 3664-64-0

(alkylaluminum chloride induced cyclization of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(alkylaluminum chloride induced cyclization of)

L18 ANSWER 31 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 92:129090 ZCA Full-text

OREF 92:21062h,21063a

TI Chemical transformations of citronellal

AU Barnes, R. A.; Goncalves, S. L.; Lago, R. C. A.; Szpiz, R. R.

CS Nucl. Pesqui. Prod. Nat., Univ. Fed. Rio de Janeiro, Rio de Janeiro, 20,000, Brazil

SO Int. Congr. Essent. Oils, [Pap.], 7th (1979), Meeting Date 1977, Volume 7, 253-6 Publisher: Japan Flavor Fragrance Manufactures' Assoc., Tokyo, Japan.

CODEN: 41XWA4

DT Conference

LA English

AB On cyclization in AcOH or reactions with Al(OCHMe2)3, MeMgI, or PhMgBr, citronellal gave I, II, Me2C:CHCH2CHg2CHMeCH2CHROH (III, R = Me, Ph), resp. Cyclization of III (R = Me, Ph) gave IV or V, resp. Me2C:CHCH2CH2CHMeCH2CH(OH)CN and Me2C:CHCH2CH2CHMeCH2CH(OAc)CN were also prepd.

ΙT 3664-64-0P

(prepn. of)

3664-64-0 ZCA RN

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

3664-64-0P ΙT (prepn. of)

L18 ANSWER 32 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 92:111168 ZCA Full-text

OREF 92:18153a,18156a

A search for new aroma chemicals - structural modification of ΤI citronellal. Part I

Sethi, V. K.; Dhar, K. L.; Atal, C. K.; Dewan, R. K. ΑU

Reg. Res. Lab., Jammu Tawi, 180001, India CS

Indian Perfumer (1978), 22(4), 225-8 SO

CODEN: IPERAS; ISSN: 0019-607X

Journal DT

English LA

Citronellal (I), isolated from Eucalyptus citriodora oil, was converted to higher homologs (II, R = Me, Et, CHMe2, R1 = H) with Grignard reactions. These were subjected to Sarett's oxidn. to give III and acetylation to give II (R1 = Ac). II (R1 = H) were hydroxylated by oxymercuration demercuration to give IV (R1 = H) which were oxidized to V and acetylated to give IV (R1 = Ac). All compds. gave different odors, with citronellyl iso-Pr ketone (III, R = CHMe2) giving the best odor.

IT 3664-64-0P

(prepn. of, for possible perfume component)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P

(prepn. of, for possible perfume component)

L18 ANSWER 33 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 86:140298 ZCA Full-text

OREF 86:22041a,22044a

TI Alkoxy substituted aliphatic di-olefinic halides

IN Henrick, Clive A.; Siddall, John B.

PA Zoecon Corp., USA

SO U.S., 14 pp. Division of U.S. 3,890,398.

CODEN: USXXAM

LA	Patent English CNT 7 PATENT NO.	KIND	DATE 	APPLICATION NO.	
PI	US 3970704			US 1975-560851	- 197503 21
	US 3729486	A	19730424	< US 1971-111650	197102 01
	US 3706733	A	19721219	< US 1971-115725	197102 16
	US 3755411	A	19730828	< US 1971-187897	197110 08
	ZA 7107375	A	19730627	< ZA 1971-7375	197111 03
	AT 319909	В	19750110	< AT 1972-316	197201 14
	US 3890398	A	19750617	< US 1972-217930	197201 14
	BE 778242	A1	19720516	< BE 1972-113026	197201 19
	SE 386161	В	19760802	< SE 1972-831	197201 25
	BR 7200434	D0	19730830	< BR 1972-434	197201 27
	IT 961136	В	19731210	< IT 1972-19871	_ :

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	RO	62490	A1	19771215	RO	1972-69767	197202 15
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	US	3803185	A	19740409	US	1972-266031	197206 26
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						<	
	US	3882156	A	19750506	US	1972-302982	197211 01
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	T. C	111161	A2	10760416	EC	<	
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PRAI		1971-111650	A2	19710201	<		
		1971-111702	A2	19710201	<		
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US 1971-111770
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CH 1972-1266
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US 1972-226147
                       19720214 <--
                  Α
US 1972-266030
                  Α2
                       19720626 <--
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AB About 30 alkatrienoic acids [Me2C:CH(CH2)2CHMeCH2CH:CHCMe:CHR (I), R = CO2Et, CO2H, CH2NH2, CH2OH, etc.] or alkadienoic acid derivs. [R1CH2CMeR2(CH2)3CHMeCH2CH:CHCMe:CHCO2R3, R1 = Cl, F, Eto, Aco; R2 = H, Cl, F; R3 = Et, H, CHMe2, K, etc.], useful as insecticides (no data), were prepd., e.g., by Wittig reaction. Thus, 1 g Me2C:CHCH2CH2CHMeCH2CHO was treated with (EtO)2P(O)CH2CMe:CHCO2Et in DMF contg. NaOEt to give I (R = CO2Et) (no yield given).

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 34 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 84:31274 ZCA Full-text

OREF 84:5125a,5128a

TI 2,4-Dienoic acid esters as insect control agents

IN Henrick, Clive A.; Siddall, John B.

PA Zoecon Corp., USA

SO U.S., 21 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 7

PATENT NO. KIND DATE APPLICATION NO. DATE

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PI	US 3912815	А	19751014	US 1974-437438	197401 28
	US 3729486	A	19730424	< US 1971-111650	197102 01
	US 3706733	А	19721219	< US 1971-115725	197102 16
	US 3755411	A	19730828	< US 1971-187897	197110 08
	ZA 7107375	A	19730627	< ZA 1971-7375	197111
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	SE 386161	В	19760802	< SE 1972-831	197201 25
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	IT 961136	В	19731210	< IT 1972-19871	197201 27
	СН 605585	A5	19780929	< CH 1975-5414	197201
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	_~				_~		197302 09
	ΑТ	7400090	A	19751115	ΑТ	< 1974-90	
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PRAI		1971-111650	A2	19710201	<		
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US 1972-226147
                     Α
                           19720214 <--
US 1972-266030
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AB About 20 Me2CR1CHR2CH2CH2CHMeCH2CH:CHCMe:CHCO2R (I, R = Et, Me, CHMe2, CH2CHMe2, CHMeEt; R1 = Cl, F, OH, OEt, OAc, cyclohexyloxy, OCHO, OMe, OCHMe2; R2 = H, Cl, F), useful as insecticides by inhibiting metamorphosis, were prepd. by addn. of R1R2 to Me2C:CHCH2CH2CHMeCH2CH:CMe:CHCO2R (II), obtained by reaction of Me2C:CHCH2CH2CHMeCH2CHO (III) with (EtO)2P(:O)CH2CMe:CHCO2R (IV). Thus, 1 g III was treated with 1.5 g IV (R = Et) in DMF contg. NaOEt to give II (R = Et), which (1 g) was hydrofluorinated in THF at 0° for 15 hr to give I (R = Et, R1 = F, R2 = H). I (R = CHMe2, R1 = OMe, R2 = H) was effective against Merchant grain beetle, almond moth, and sawtoothed grain beetle.

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 35 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 84:31273 ZCA Full-text

OREF 84:5125a,5128a

TI 2,4-Dienoic acids, esters, and derivatives

IN Henrick, Clive A.; Siddall, John B.

PA Zoecon Corp., USA

SO U.S., 21 pp. CODEN: USXXAM

DT Patent

LA English

FAN	.CNT 7				
	PATENT NO.		DATE 	APPLICATION NO.	DATE 
ΡI	US 3904662	А	19750909	US 1972-263903	10000
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	US 3706733	А	19721219	US 1971-115725	197102
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US	3838176	А	19740924	US	< 1972-281885	18 197208
US	3882156	A	19750506	US	< 1972-302982	18 197211
BE	791621	A4	19730521	BE	< 1972-124362	01
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PRAI US	1971-111650	A2	19710201 <	<	<	

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AB About 30 Me2CR1CHR2CH2CH2CHMeCH2CH:CHCMe:CHCO2R (I, R = Et, H, CMe3, CHMe2, CH2CHMe2, CHMeEt, CH2CH:CHMe, CH2CH:CH2, CH2CH2CH:CH2, CHMeCH:CH2, CH2C.tplbond.CH, cyclopropyl, cyclopentyl; R1 = F, Cl, OH, OEt, OAc, OMe, OCHO, OCHMe2; R2 = H, Cl, F), useful for control of peach aphid, Indian meal moth, Merchant grain beetle, and almond moth by inhibiting metamorphosis, were prepd. by addn. of R1R2 to Me2C:CHCH2CH2CHMeCH2CH:CHCMe:CHCO2R (II), obtained by reaction of Me2C:CHCH2CH2CHMeCH2CHO (III) with (EtO)2P(:O)CH2CMe:CHCO2R (IV). Thus, 1 g III was treated with 1.5 g IV (R = Et) in DMF contg. NaOEt to give II (R = Et), which (1 g) was hydrofluorinated in THF at 0° for 15 hr to give I (R = Et, R1 = F, R2 = H).

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 36 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 83:43514 ZCA Full-text

OREF 83:6899a,6902a

TI Synthesis and physiological tests of substances possessing insect juvenile hormone activity

AU Kuznetsov, N. V.; Guznenok, N. Kh.; Myrsina, R. A.; Svishchuk, A. A.

CS Inst. Org. Khim., Kiev, USSR

SO Fiziologicheski Aktivnye Veshchestva (1966-1992) (1974), 6, 105-10

CODEN: FAVUAI; ISSN: 0533-1153

DT Journal

LA Russian

GI For diagram(s), see printed CA Issue.

AB Sesquiterpenoids possessing insect juvenile hormone activity, e.g. I [R1 = Me, R2 = Me, Et, R3 = Me2C:CHCH2CH2, H[CH2CMe:CH2CH2]2CH2] were obtained in 34-42% yields by Grignard reactions of esters II (R1 = H, Me). Addnl. obtained were 12 esters and ketones which had activities of 0.05  $\mu$ g/pupa for I (R1 = Me, R2 = Et, R3 = Me2C:CHCH2CH2) to 250 mg/pupa for Me2C:CHCH2CH2CMe:CHCH2CH2COMe. Grignard reactions of I led to R1COCH:CR2R3[R1 = Me, H, R2 = Me, Et, R3 = Me, MeC6H4, Me2C:CHCH2CH2, C9H19, EtMeC:CHCH2CH2, H[CH2MeC:CHCH2CH2]2CH2, H[CH2EtC:CHCH2CH2]2CH2].

IT 3664-64-0

(juvenile hormone activity of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(juvenile hormone activity of)

L18 ANSWER 37 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 78:110626 ZCA Full-text

OREF 78:17758h,17759a

TI Aliphatic unsaturated compounds and their insecticidal compositions

IN Henrick, Clive A.; Siddall, John B.

PA Zoecon Corp.

SO Ger. Offen., 113 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 7

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	1972-1266	A	19720120			
	1972-226147	A A2	19720214			
	large no. of ethyl				general formula·	
	_		<del>-</del>	_	n = 0-3, $R = F$	R5R6C•CR7
					or alkyl; $R8$ , $R9 = F$	
01		~ _ 1. 7	=, =:0, =:1			-, <i></i> , <i></i> ,

F, OH, acyloxy, hydrocarbyloxy); R1, R4 = lower alkyl; R2, R3 = H or lower alkyl; R5 = CO2R10, COR10, C(O)SR10, COX, CH2X, etc., where R10 = H or hydrocarbyl, X = Br, Cl, or F] were prepd. and were effective insecticides. Thus, 1 g Me2C:CHCH2CH2CHMeCH2CHO and 1.5 g EtO2CCH:CMeCH2P(O)(OEt)2 reacted in DMF in the presence of EtONa to give (E,E)-I (m = n = 1; R = Me2C:CH2, R1 = R4 = Me, R2 = R3 = H, R5 = CO2Et), which killed Aedes aegypti at 1 ppm for ID50.

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 38 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 72:21261 ZCA Full-text

OREF 72:3869a,3872a

TI Addition of Grignard reagents based on the double bond of crotonic acid esters and ethylidene acetone

AU Kuznetsov, N. V.; Guznenok, N. Kh.

CS Inst. Org. Khim., Kiev, USSR

SO Dopovidi Akademii Nauk Ukrains'koi RSR, Seriya B: Geologiya, Geofizika, Khimiya ta Biologiya (1969), 31(10), 908-10 CODEN: DBGGAM; ISSN: 0002-3523

DT Journal

LA Ukrainian

GI For diagram(s), see printed CA Issue.

AB Esters of d,l-citronellic acid (I) were obtained by a general method exemplified by the following procedure: 1.25 g iso-Pr crotonate in 10 ml Et20 was added at -5° over 3 hr to a Grignard soln. prepd. from 5.25 g 5-bromo-2-methyl-2-pentene (II), 0.6 g Mg, and 8 ml Et20. In the case of Et crotonate and ethylideneacetone (III) the reactions were carried out in the presence of 0.1 g Cu2Cl2. Conventional workup gave 50-70% I esters, sapon. of which with alc. NaO H gave 70% I, b10 144-5°, n15D 1.4630. Grignard reagents obtained from II, PhBr, and iso-C5H11Br add far more readily to et ethylideneacetoacetate ester (IV) than to alkyl croto nates and III. Thus, 7.8 g IV (prepn. described) was added dropwise to the Grignard reagent obtained from 1.2 g Mg, 7.8 g PhBr, and 40 ml Et20, at <-10°, and the mixt. was

kept 1 hr  $<-10^{\circ}$  and worked up to give Et 2-acetyl-3-phenylbutyrate. Grignard reagents did not add to cyclic unsatd. esters. The phys. consts. of R1CHMeCHR2COR3 obtained are shown in the table.

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 39 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 68:95127 ZCA Full-text

OREF 68:18311a,18314a

TI Thermal cyclization of  $\varepsilon$ ,  $\zeta$ -unsaturated ketones

AU Le Perchec, Pierre

CS Fac. Sci. Caen, Caen, Fr.

SO Annales de Chimie (Paris, France) (1967), 2(5), 263-8 CODEN: ANCPAC; ISSN: 0151-9107

DT Journal

LA French

The thermal cyclization of  $\epsilon$ ,  $\zeta$ -unsatd. ketones was investigated. Heating 7-octen-2-one (I) for 30 min. in a sealed tube at 370° gave a 93:7 mixt. of trans-2- methylacetylcyclopentane and the cis isomer. Other ketones were thermally cyclized in a similar manner [starting material and product(s) given]: 3-methyl-7-octen-2-one, trans-1,2-dimethyl- acetylcyclopentane; 7-methyl-7-octen-2-one, 2,2-dimethylacetyl- cyclopentane; 7-methyl-7-octen-2-one, 2,2-dimethylacetyl- cyclopentane; 7-methyl-7-octen-2-one, 2,2-dimethylacetylcyclopentane;

4,8-dimethyl-7-nonen-2-one, 2-isopropyl-5-methylcyclopentane and 2,4-dimethylcumene; 3-carbethoxy-7-octen-2-one, trans-1-carbethoxy-2-methylacetylcyclopentane; and 6-benzoyl-1-heptene, trans-1,2-dimethylbenzoylcyclopentane. Similar treatment of 3-carbethoxy-3-methyl-7-octen-2-one gave trans-1,2-dimethylacetylcyclopentane by decarboxylation. Similar heating of the enol acetate, the ethylene ketal, the di-Me ketal, the di-Et ketal, and the corresponding enol ethers of I also gave the thermocyclization ketone. The cis stereochemistry for the thermocyclization for  $\epsilon,\zeta$ -unsatd. ketones, the thermocyclization of  $\alpha$ -deuterated  $\epsilon,\zeta$ -unsatd. ketones, the 1st

order rate const. for this reaction, and the migration of the Me group in the thermal cyclization of Me enol ethers of I support an intramol. mechanism involving transfer of the enol H to the terminal methylene group and the ring-closing formation of the  $\alpha,\epsilon$ -bond. Thermal rearrangements of  $\alpha$ -allyl- $\beta,\gamma$ -unsatd. ketones involve 2 steps, i.e. Cope rearrangement followed by thermal cyclization of the  $\alpha,\beta\colon$   $\epsilon,\zeta$ -unsatd. ketones formed.

IT 3664-64-0

(ring closure of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0

(ring closure of)

L18 ANSWER 40 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 67:53740 ZCA Full-text

OREF 67:10071a,10074a

TI Thermolysis and photolysis of unsaturated ketones.V. Thermal cyclization of aliphatic  $\epsilon,\zeta$ -ethylenic ketones

AU Rouessac, Francis; Le Perchec, Pierre; Conia, Jean M.

CS Fac. Sci. Caen, Caen, Fr.

SO Bulletin de la Societe Chimique de France (1967), (3), 818-22

CODEN: BSCFAS; ISSN: 0037-8968

DT Journal

LA French

OS CASREACT 67:53740

GI For diagram(s), see printed CA Issue.

AB cf. CA 65: 13563b. Compds. of the general formula AcCHRCHR1CH2CH2CR2:CR32, where R, R1, and R2 are H, Me, or CO2Et and R3 is H or Me, are heated to give 2-alkyl-1-acetylcyclopentanes by the mechanism shown. Thus, AcCH2CO2Et is treated with CH2:CH(CH2)3Br in the presence of NaOEt to give 3-carbethoxy-7-octen-2-one (I), b20 120-2°, n20D 1.4408. Decarboethoxylation (Le Bel, et al, CA 61:10671a) of I gives 78% 7-octen-2-one, b. 176°, n20D 1.4250. 7-Octen-2-one is heated to give .apprx.90% mixt. contg. 7% cis-2-methylacetylcyclopentane, n22.5D 1.4455, and 93% trans-2-methylacetylcyclopentane, n21D 1.4390. Similarly prepd. are (alkenone reactant given): 1-carboethoxy-2-methylacetylcyclopentane (II) (n23D

1.4502), I; trans-1,2- dimethylacetylcyclopentane (III) (n19.5D 1.4493; 2,4-dinitrophenylhydrazone m. 115-16°), 3-methyl-7-octen-2-one; 2,2-dimethylacetylcyclopentane (semicarbazone m. 173°), 7-methyl-7-octen-2-one; a mixt. of 2,4-dimethylcumene and 2-isopropyl-5-methylacetylcyclopentane isomers (n18D 1.4526), 4,8-dimethyl-7-nonen-2-one (IV); trans-1,2-dimethyl - 1 - benzoylcyclopentane (2,4-dinitrophenylhydrazone m. 143°), 6-benzoyl-1-heptene. II is heated 2 hrs. at 40° with 400 mg. NaOH in 10 ml. water to give trans-2-methylacetylcyclopentane. III is treated with NaOI to give trans-1,2-dimethylcyclopentanecarboxyli c acid, m. 46° (amide m. 98°). Also prepd. are (b.p./mm., n25D, and m.p. 2,4-dinitrophenylhydrazone given): 3-methyl-7-octen-2-one, 182°/760, 1.4300, 43°; 7-methyl-7-octen-2-one, - (n23D 1.4370), 58°; IV, -, -, 61°; 6-benzoyl-1-heptene, 90-3°/0.15, -, 81°.

IT 3664-64-0P

(prepn. of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0P (prepn. of)

L18 ANSWER 41 OF 41 ZCA COPYRIGHT 2008 ACS on STN

AN 63:88482 ZCA Full-text

OREF 63:16223a-e

TI Thermal cyclization of  $\varepsilon$ ,  $\zeta$ -ethylenic ketones

AU Rouessac, Francis; Conia, Jean Marie

CS Univ. Caen, Fr.

SO Tetrahedron Letters (1965), (37), 3313-18 CODEN: TELEAY; ISSN: 0040-4039

DT Journal

LA French

GI For diagram(s), see printed CA Issue.

The monoethylenic ketones (I, all groups H) (II); (I, all groups H except R1 = Me) (III); (I, all groups H except R1 = CO2Et) (IV); (I, all groups H except R3 = Me) (V); (I, all groups H except R2 = R4 = R5 = Me) (VI) heated in sealed pyrex tubes and the products sepd. by vapor phase chromatography gave 1-acetyl-2-alkylcyclopentanes (VII). Treatment of AcCH2CO2Et with BrCH2CH2CH2CH:CH2 in the presence of NaOEt gave IV, b20  $120-2^{\circ}$ , v 1735, 1710 cm.-1, de-carboxylated to II,

b. 176°,  $\delta$  2.02 ppm. [dinitrophenylhydrazone (DNP) m. 64°]. Methylation of IV gave 3-carbethoxy-3-methyl-7-octen-2-one (VIII), b20 130°,  $\nu$  1730, 1710 cm.-1,  $\delta$  2.03, 1.24 ppm., converted by alk. decarbethoxylation to III, b. 182°, 1.04 ppm. (J 6 cycles/sec.); DNP, m. 42°. II, III, IV, and VIII gave intense N.M.R. peaks between 4.70 and 6.10 ppm. characteristic of allyl group olefinic protons, absent in the cyclic VII. Wittig reaction between 2,7-octanedione and Ph3PMeBr gave V,  $\delta$  1.69, 4.64 ppm. (DNP m. 58°). Treatment of citronellal with MeMgI and oxidn. of the 4,8-dimethyl-2-hydroxy-7nonene with CrO3-C5H5N gave VI, b16 102°,  $\delta$  0.92, 5.27 ppm. (DNP m. 61°). II heated 2 hrs. at 330° or 30 min. at 370° gave a quant. yield of a mixt. of 5-7% cis-2-methyl-1-acetyleyclopentane,  $\delta$  0.81 ppm. (J 6.0 cycles/sec.) (DNP m.  $117^{\circ}$ ); and 93-5% trans-2-methyl-1acetylcyclopentane,  $\delta$  1.01 (J 6.5 cycles/ sec.) (DNF m. 109°). III heated 30 min. at 370° gave a quant. yield of trans-1,2-dimethyl-1acetyl-cyclopentane (IX),  $\delta$  0.86, 1.20, 2.03 ppm. (DNP m. 116°). IX treated with NaOBr gave an acid, characterized as amide, m. 98°. IV heated 20 hrs. at 250° or 1 hr. at 300° gave quant. 1-carbethoxy-2methyl-1-acetylcyclopentane, v 1735, 1705 cm.-1  $\delta$  0.90 ppm., decarbethoxylated to the same mixt. as obtained by thermal cyclization of II. V heated 2 hrs. at 330° gave the known 2,2dimethyl-1-acetylcyclopentane,  $\delta$  0.86, 1.19, 2.05 ppm.; semicarbazone m. 173°. VI heated under similar conditions gave 60% yields of ketones, consisting mainly of stereoisomeric 2-isopropyl-5-methyl-1acetylcyclopentanes,  $\delta$  2.07, 1.01, 0.80, 0.87 ppm.

IT 3664-64-0, 7-Nonen-2-one, 4,8-dimethyl-(cyclization of)

RN 3664-64-0 ZCA

CN 7-Nonen-2-one, 4,8-dimethyl- (CA INDEX NAME)

IT 3664-64-0, 7-Nonen-2-one, 4,8-dimethyl-(cyclization of)